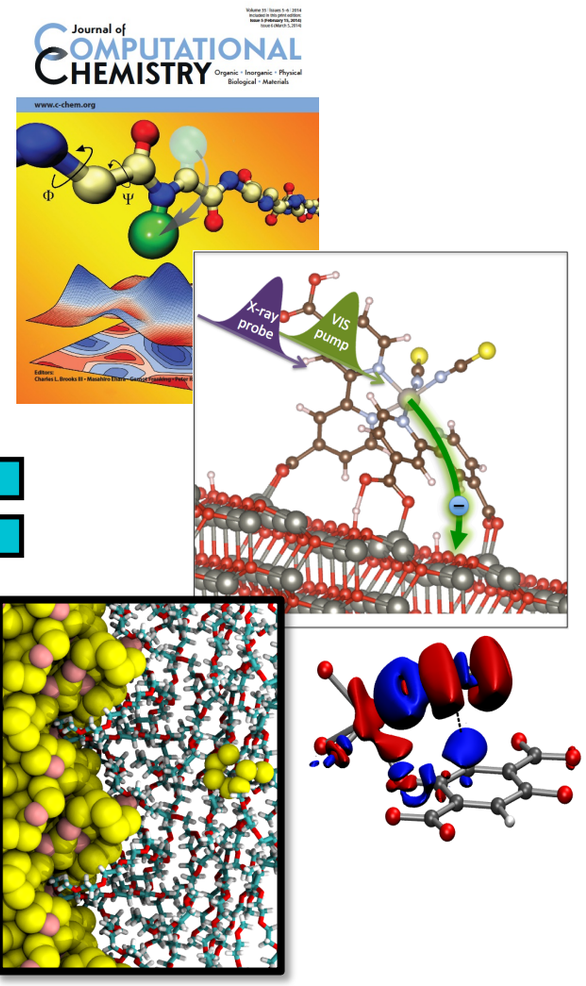
Molecular Foundry

NCEM NATIONAL CENTER FOR ELECTRON MICROSCOPY

BERKELEY LAB
Lawrence Berkeley National Laboratory

High Performance Computing at The Molecular Foundry



David Prendergast
Theory of Nanostructured Materials Facility
The Molecular Foundry
dgprendergast@lbl.gov

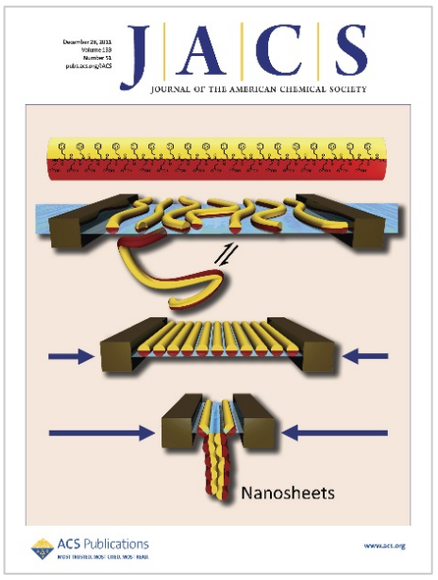
LabTech2014
September 10, 2014

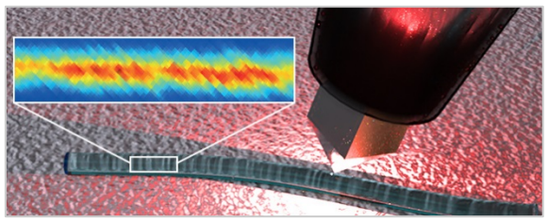
U.S. DEPARTMENT OF ENERGY

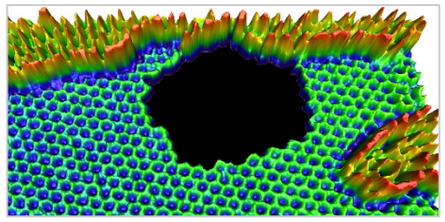
Molecular Foundry

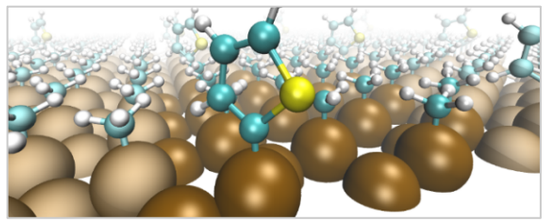
A Knowledge-Based User Facility for Nanoscale Science

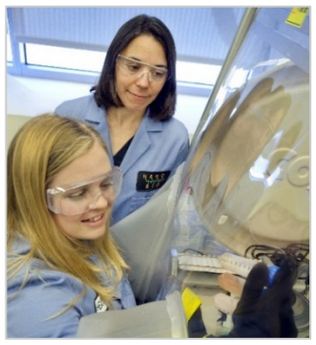
- **Knowledge-based user facility** that provides state-of-the-art expertise and instrumentation in nanoscale science in a safe environment
- **Multidisciplinary research institute** at the forefront of nanoscale science

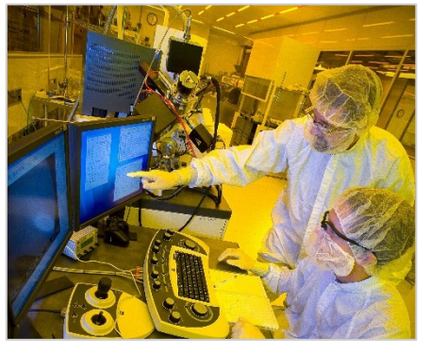


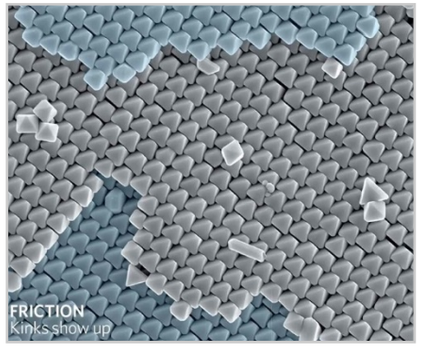


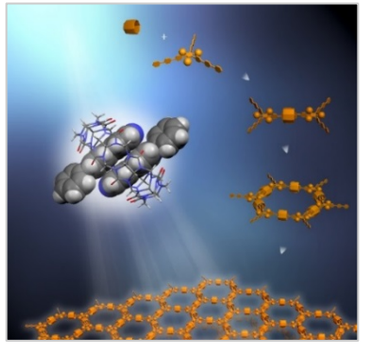












Foundry Expertise & the 50/50 Model

Molecular Foundry

29 PI staff scientists + 18 technical staff

NCEM

Molecular Foundry Scientific Organization

National Center for Electron Microscopy (NCEM)
Electron microscopy and nanocharacterization

Organic and Macromolecular Synthesis
Soft materials: organics, macromolecules, polymers and their assemblies

Biological Nanostructures
New bio-materials; new probes for bio-imaging; synthetic biology techniques

Inorganic Nanostructures
Science of semiconductor, carbon and hybrid nanostructures

Theory of Nanostructured Materials
Studies to guide understanding of new principles, behavior and experiments

Nanofabrication
Advanced lithographic and thin-film processing techniques

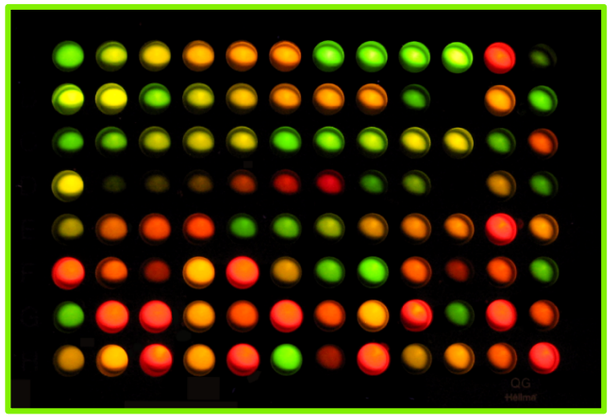
Imaging and Manipulation of Nanostructures
Characterization and manipulation of nanostructures

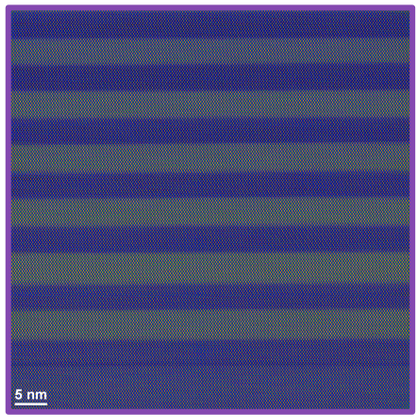
Molecular Foundry

NCEM

Scientific Research Themes

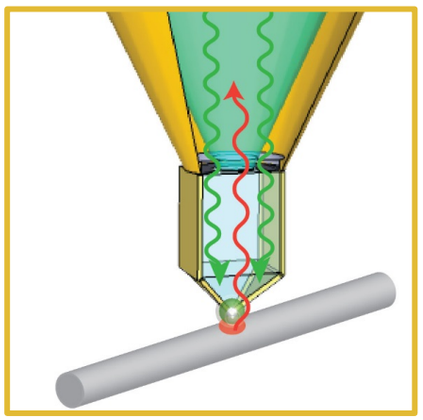
Combinatorial Nanoscience

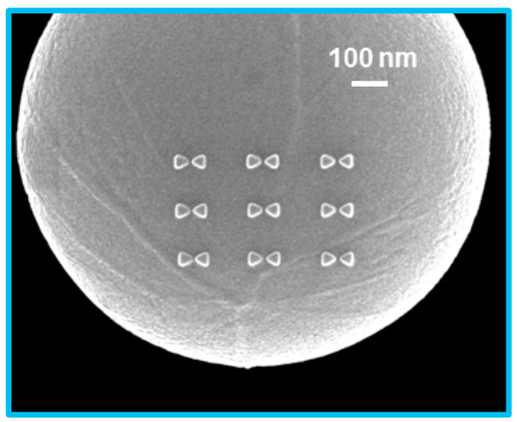




Functional Nanointerfaces

Multimodal Nanoscale Imaging





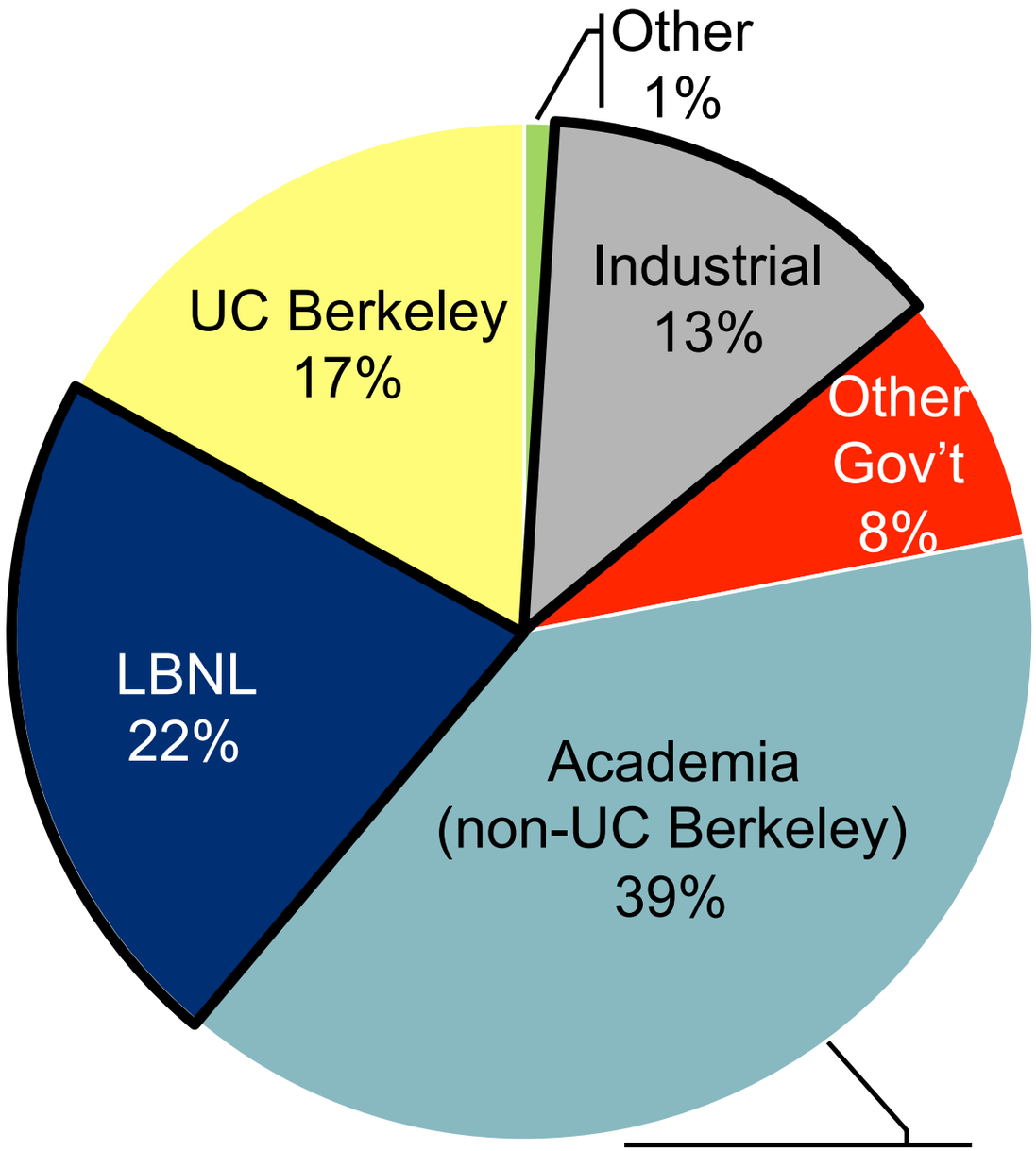
Single-Digit Nanofabrication and Assembly

Molecular Foundry

NCEM

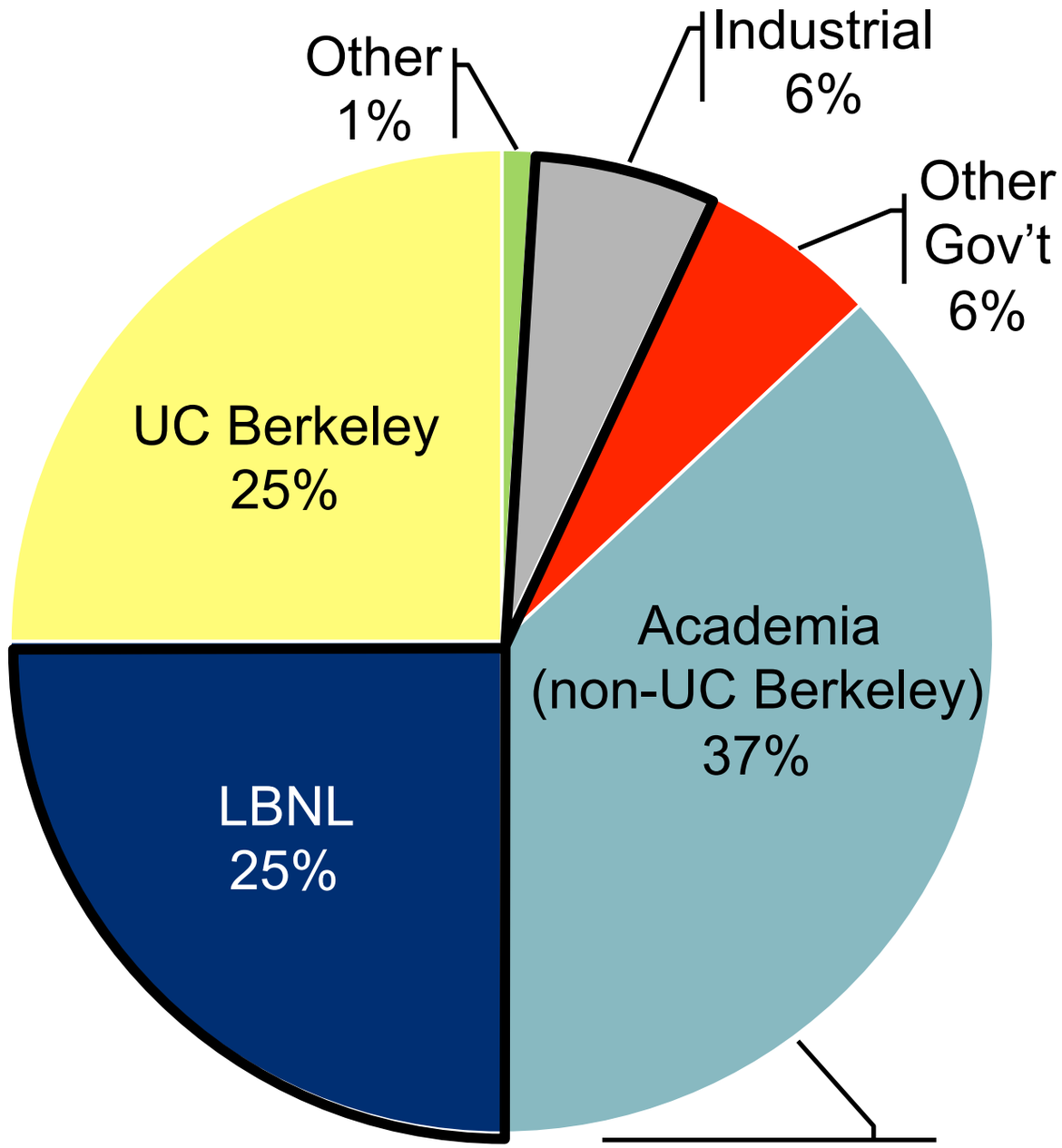
User Demographics: FY10-present

Molecular Foundry



40 states + DC
36 foreign countries

NCEM



33 states + DC & PR
21 foreign countries

Recent Industry Users

aBeam technologies

HGST a Western Digital company

Kiverdi

Abbott A Promise for Life

heliotrope

Blue Planet Co.,Ltd. http://www.blueplanet.co.kr

ELECTRON OPTICA

Matrix Sensors

Nanotech Bio

APPLIED MATERIALS®

Seagate®

FEI™

DOW®

Chevron

Pfizer

TOYOTA

gatan

micro resist technology

Protochips Quantifiably Better™

Newomics

DUPONT

Porifera

molecular VISTA

Genentech

Pacific Light Technologies

inpria INORGANIC PRINTED ELECTRONICS

GM

intel®

Alveo Energy

HUMMINGBIRD SCIENTIFIC

MERCK Research Laboratories

PLANT PV New Materials for Photovoltaic Cells

nano Hydrophobics, Inc.

eSionic

HALDOR TOPSOE CATALYSING YOUR BUSINESS

P-BLiNC Portable BioLab in a NanoChip

EVOSOL

SEMATECH

HYSITRON®

Molecular Foundry

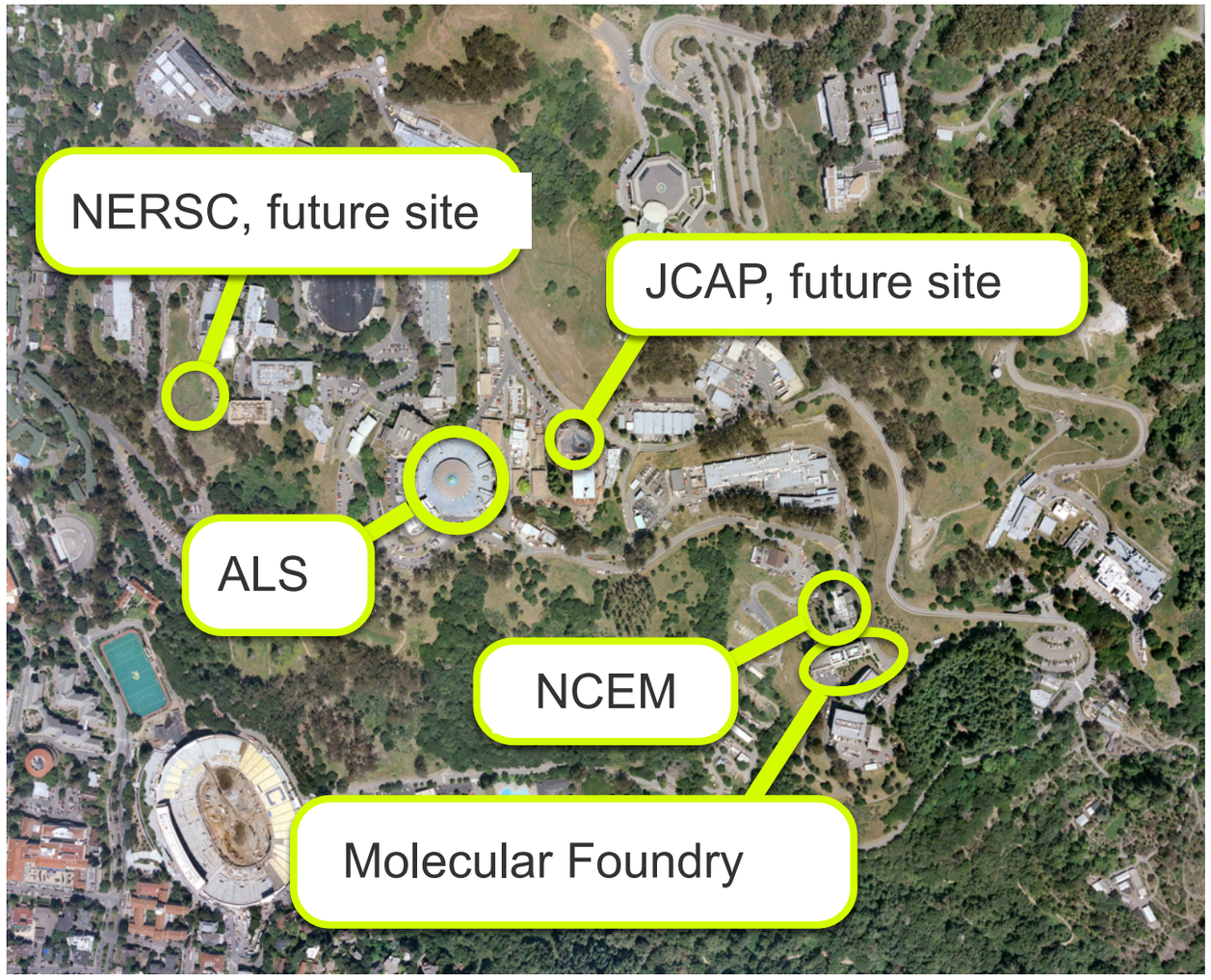
NCEM

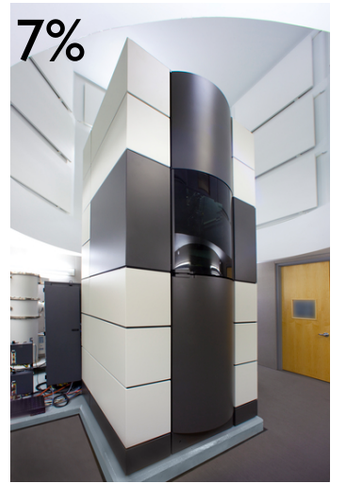
Connection to Other Parts of LBNL

Over 37% of Molecular Foundry publications involve use of other LBNL user facilities and programs (FY12-current)

Advanced Light Source (ALS)

National Energy Research Scientific Computing Center (NERSC)





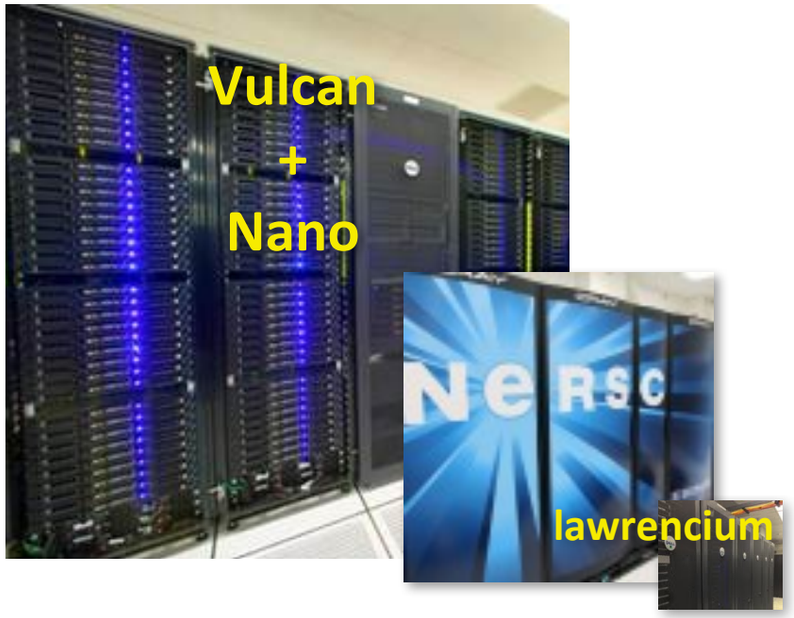
National Center for Electron Microscopy (NCEM)

Other LBNL programs

Molecular Foundry

NCEM

High Performance Computing Services (HPCS) and dedicated compute clusters



22M CPUhrs 6M <1M

24/7 access to dedicated resources vital for development and application

Test-bed for new technology

courtesy: Gary Jung, HPCS

Molecular Foundry

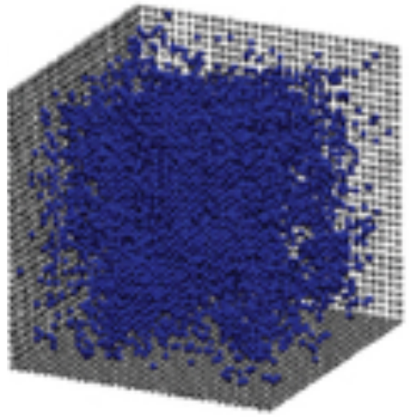
NVIDIA

NCEM

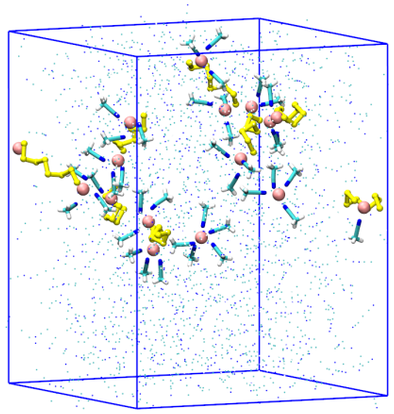
Theory of Nanostructured Materials Facility

… from electrons to assemblies

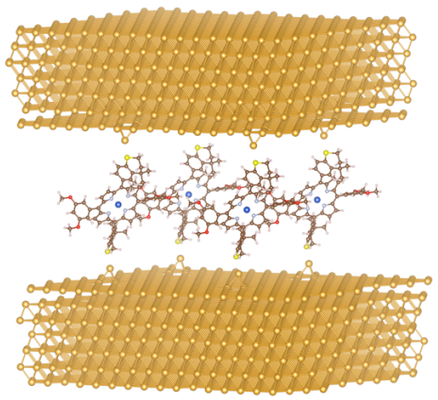
Developing fundamental understanding of energy-relevant phenomena and materials at the nanoscale, with a focus on electronic transport, computational spectroscopy, and self-assembly.



Statistical mechanics
Ab initio forcefield development
Coarse-grained modeling
Whitelam



Electronic core-level excitations
Molecular Dynamics
Simulated X-ray Spectroscopy
Prendergast



Electronic excited state methos
Electron transport
Weak interactions
Neaton

Recognized hard problems:
Weak interactions
Strong correlations
Excited states and dynamics
Nonequilibrium phenomena
Self-assembly and growth

time

length

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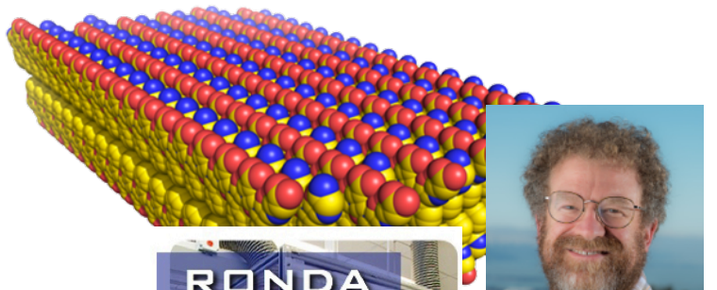
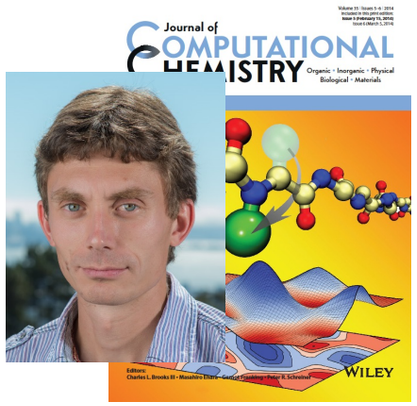
Modeling Biomimetic Polymer Self-Assembly



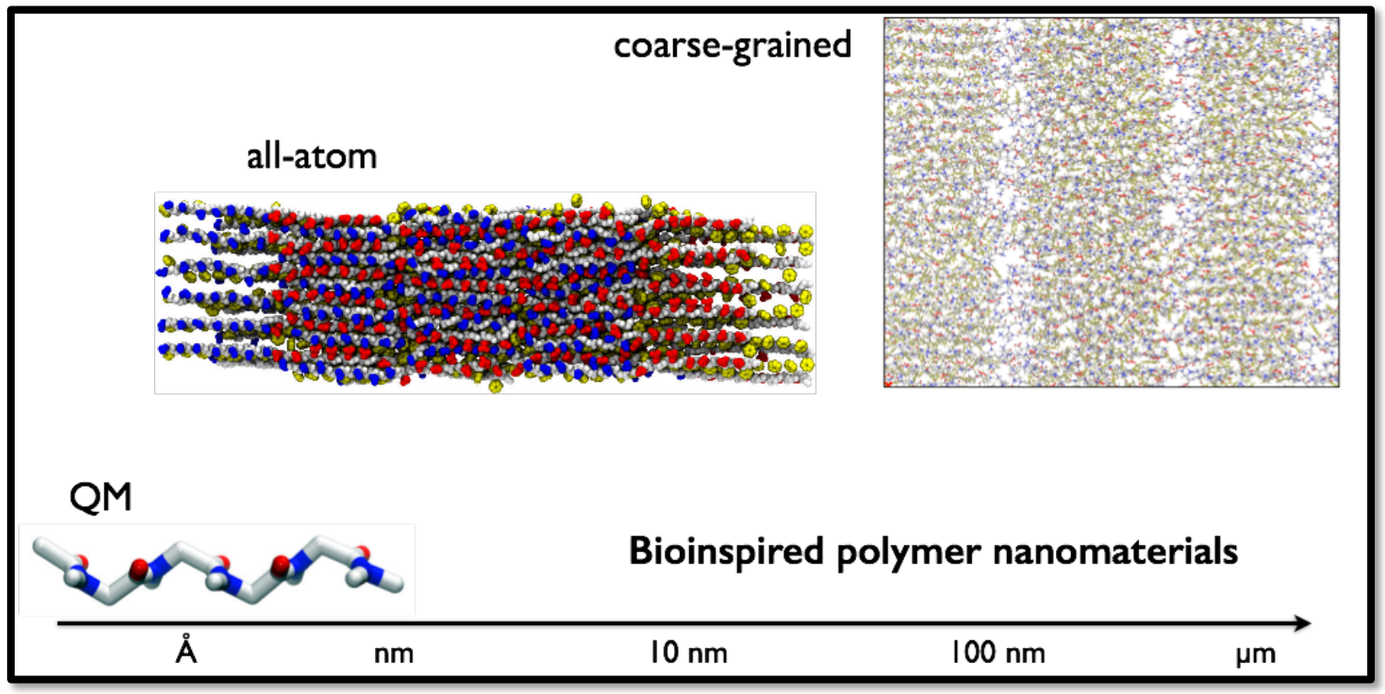
Automated Biopolymer Synthesis Robots

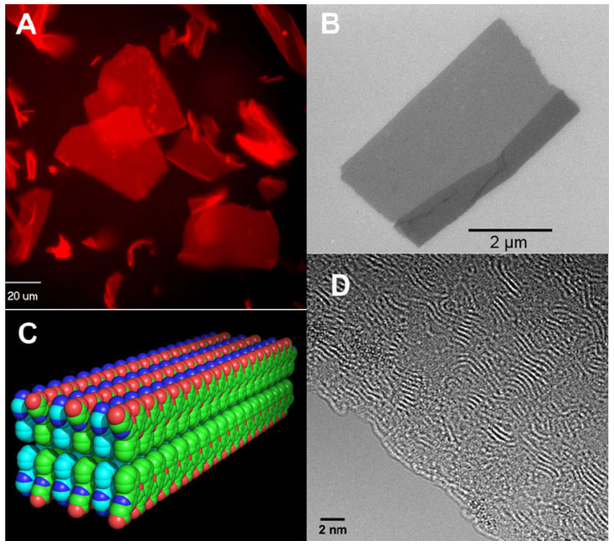
Foundry staff Ron Zuckermann



New Force-Fields for Peptoid Simulation

Foundry staff Steve Whitelam





ALS

X-ray Scattering and Spectroscopy

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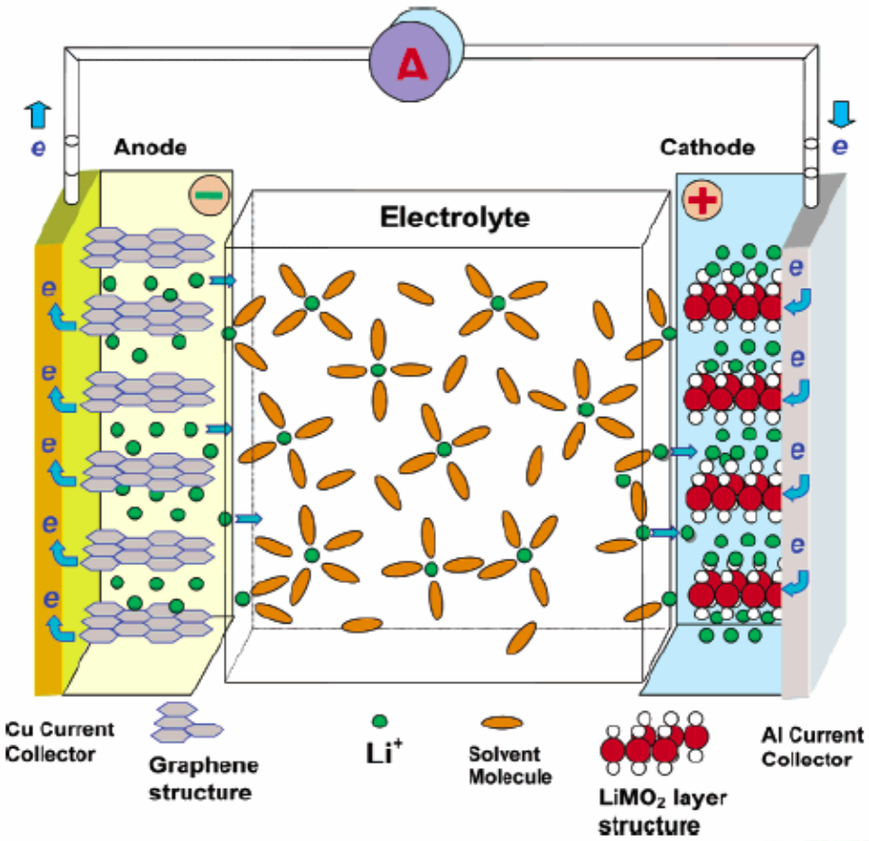
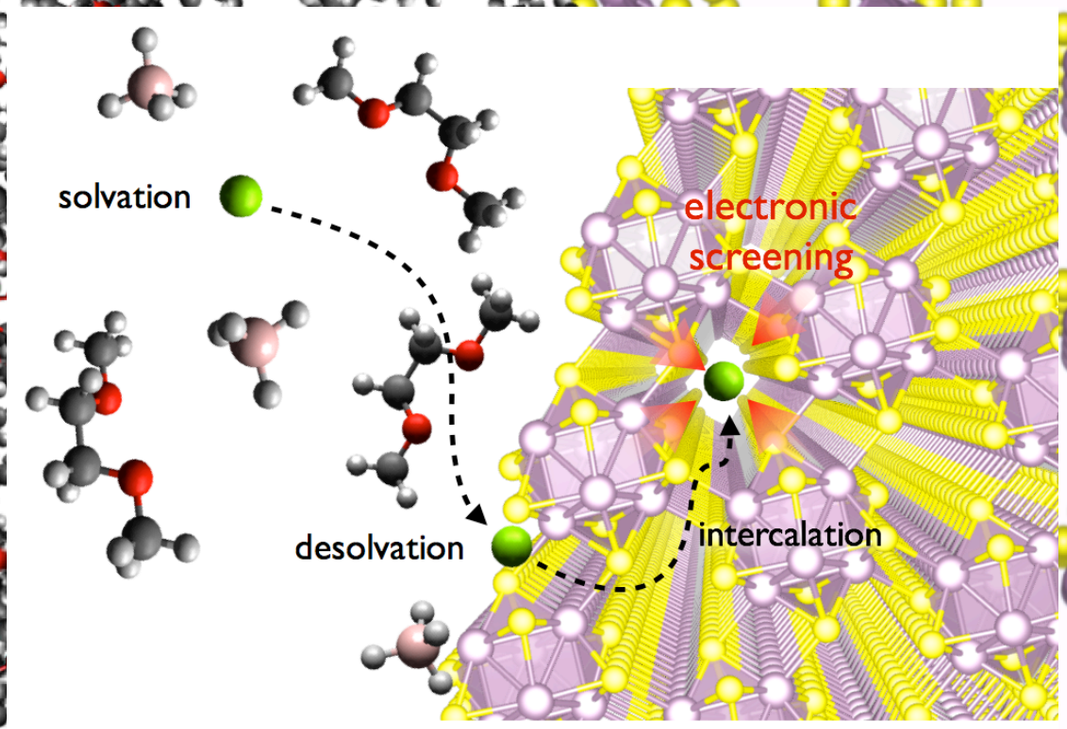
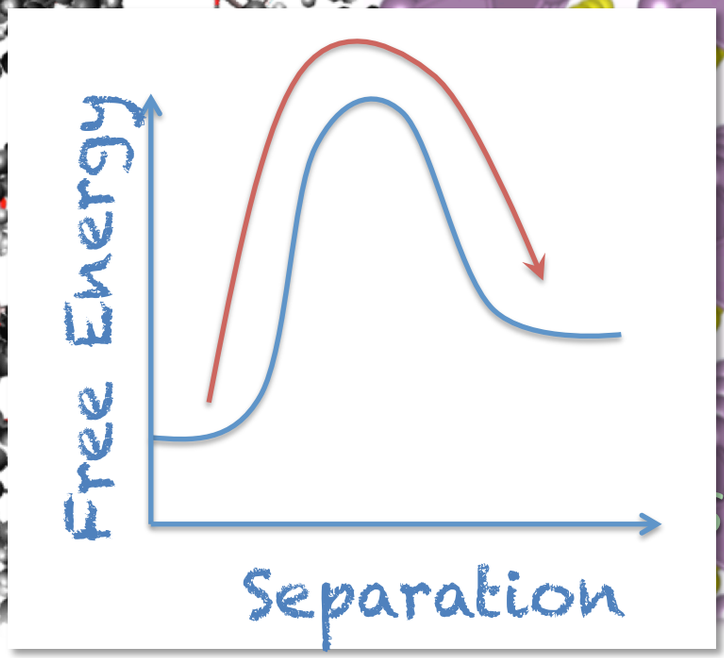
NCEM

Battery Function at Working Interfaces





Charge Dynamics
Molecular Dynamics (ab initio)
Free Energy Sampling
Strongly Correlated Electrons
…



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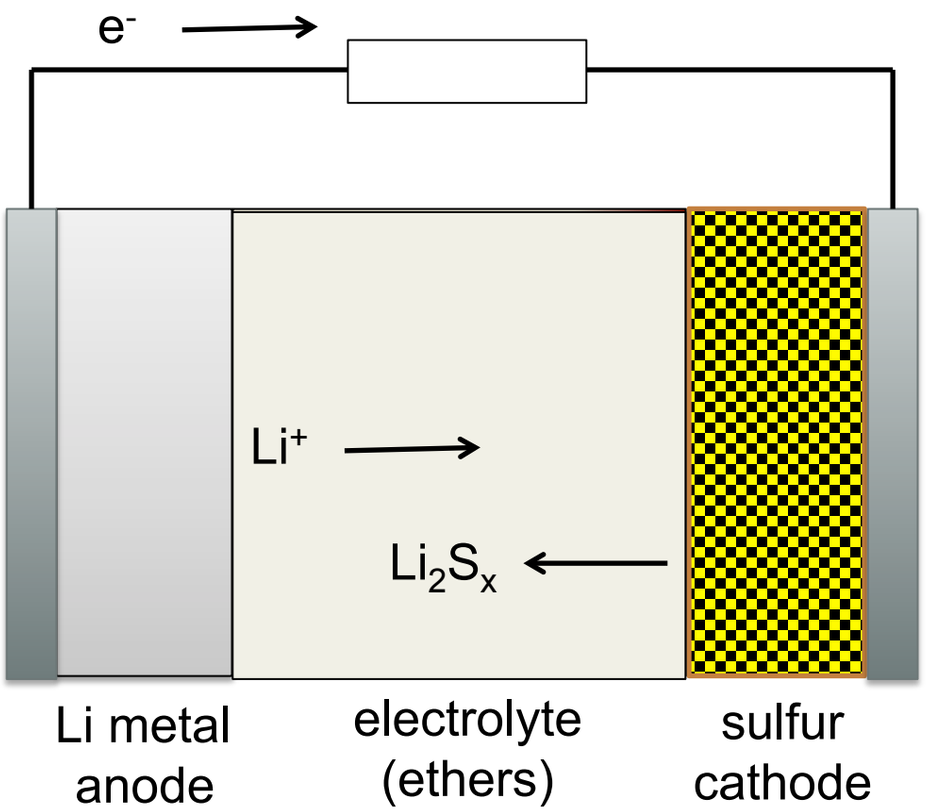
Sabrina Wan

BERKELEY LAB

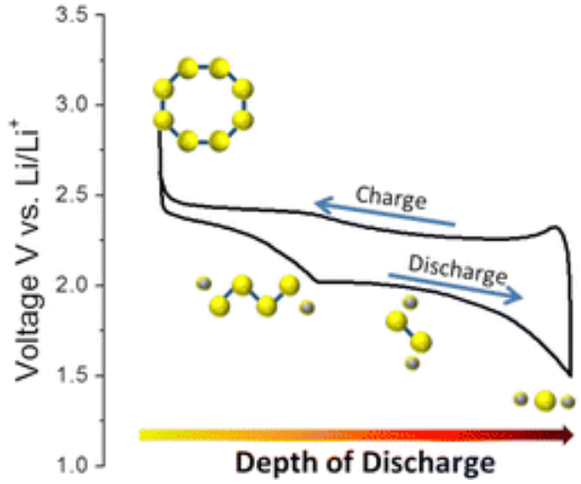
Typical demise of lithium-sulfur battery



- Discharge: $16Li^+ + 16e^- + S_8 \rightarrow 8Li_2S$
- Stepwise(?): $2Li^+ + 2e^- + S_8 \rightarrow Li_2S_8$
  … Li_2S_6, Li_2S_4, Li_2S_2
  … LiS_3 (radicals)

Li-S batteries Issues

- Both Li_2S and S_8 are insulators – conducting contact
- Multi-step reactions at cathode: creates various Li_2S_x



Evers, Nazar, Acc. Chem. Res.(2012)

- Li_2S_x species are soluble in electrolyte
- Parasitic shuttle reactions at anode

Problem: Loss of active cathode material
Infinite charging

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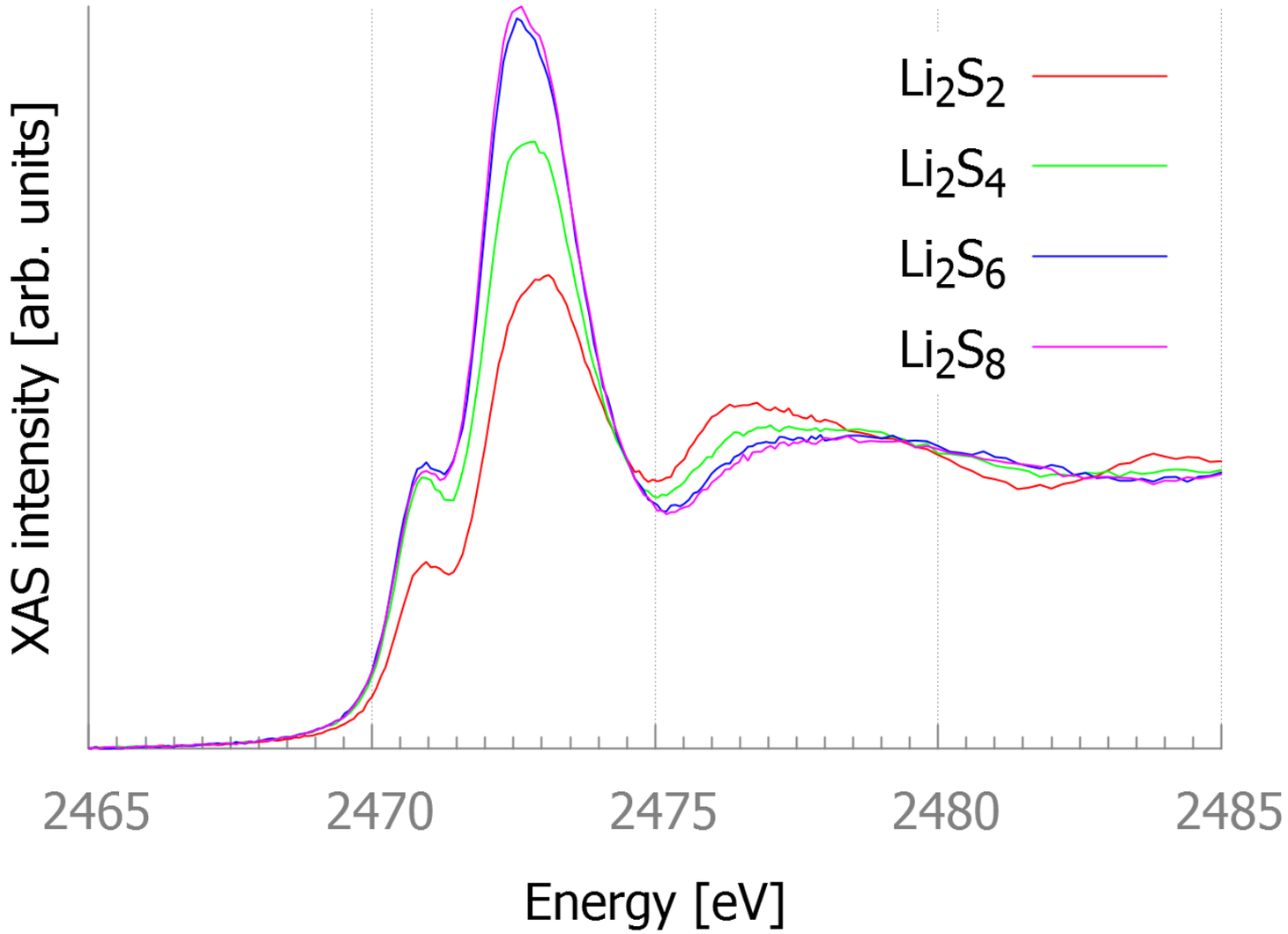
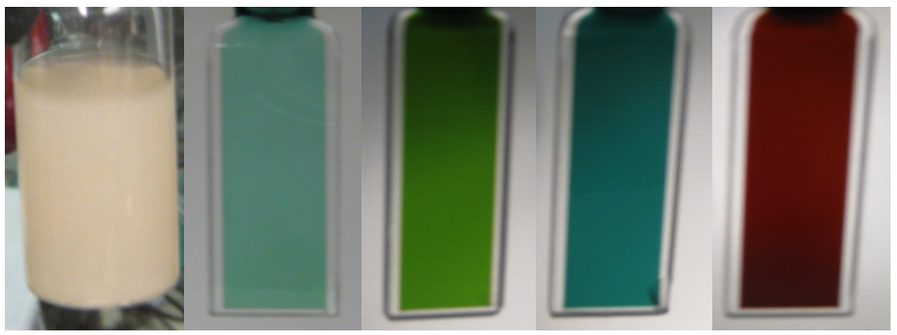
Experimental S K-edge XAS spectra of Li_2S_x dissolved in polyglymes



Stoichiometric mixtures of sulfur (S_8) and lithium sulfide (Li_2S)

$Li_2S + (x-1)/8\ S_8 \rightarrow Li_2S_x$



Can we associate a given spectral fingerprint (color of XAS) with the existence of the corresponding molecular species?

Measurements by Kevin Wujcik et al. (Balsara Group)

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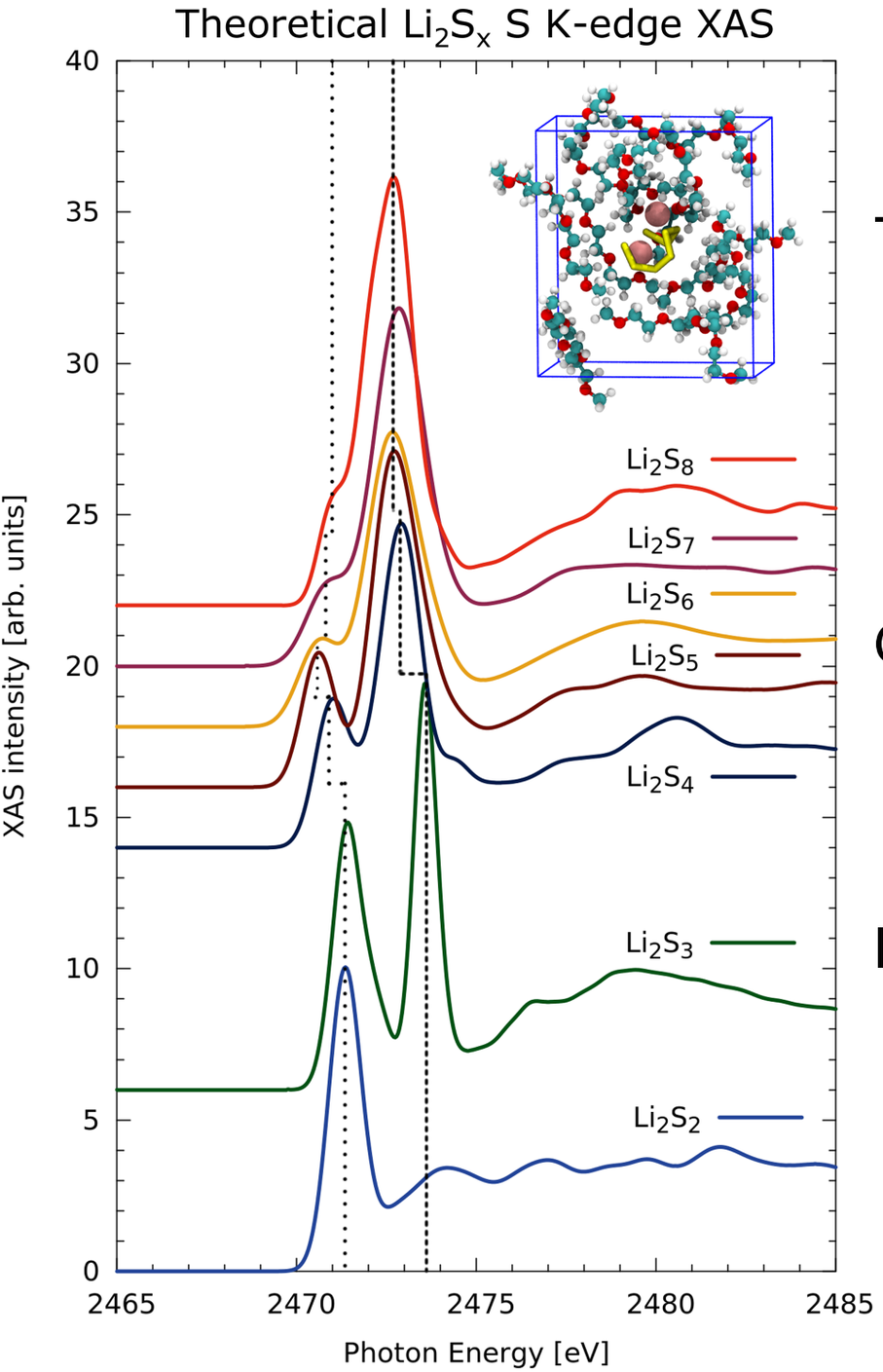
Conclusions:
S K-edge XAS of Li_2S_x in TEGDME



Two main features:

pre-edge – **terminal sulfur atoms**

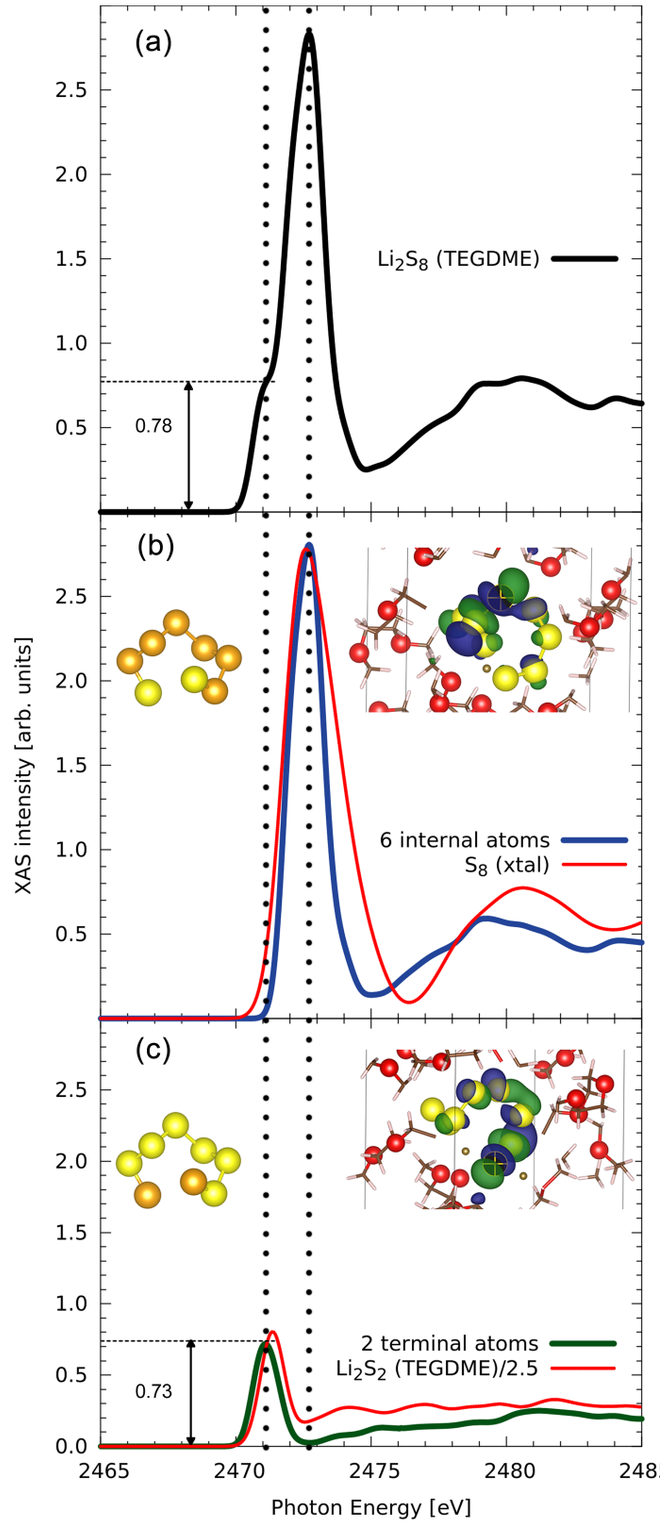
main-edge – **internal sulfur atoms**

General red-shift with increasing length

Increasing S-S bond lengths

Increase in intensity ratio

More internal -S- atoms



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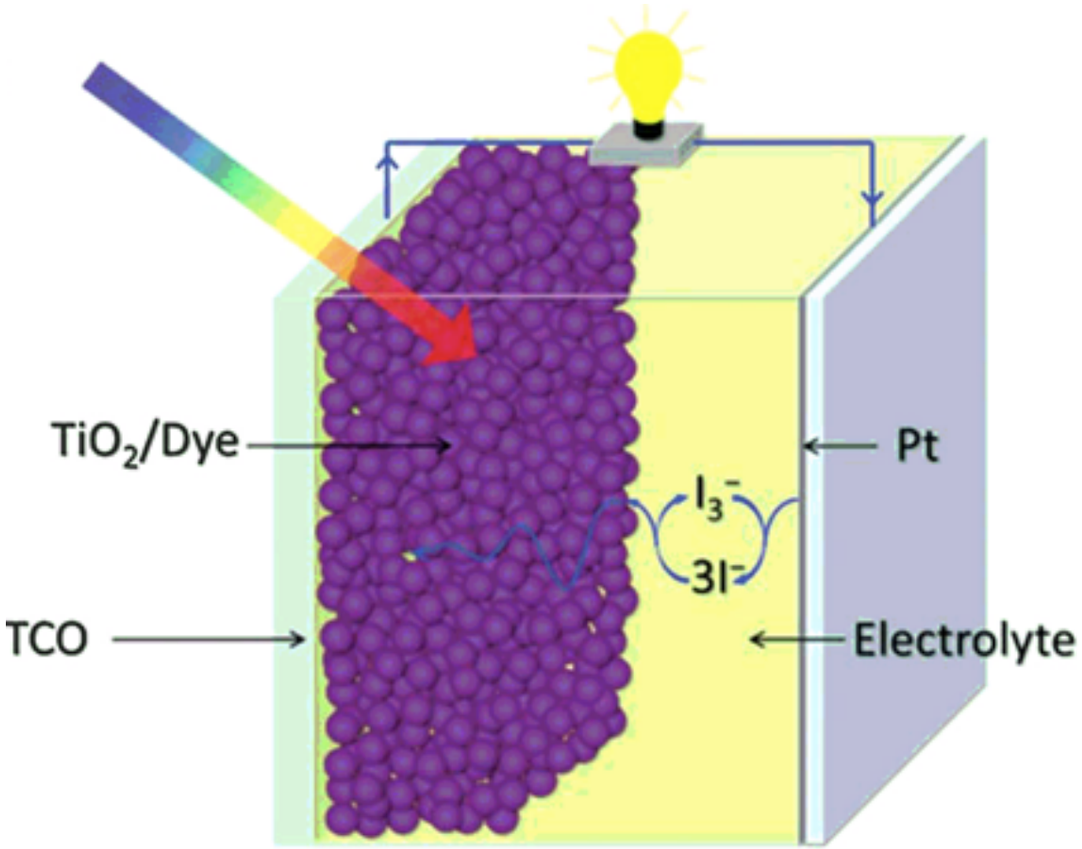
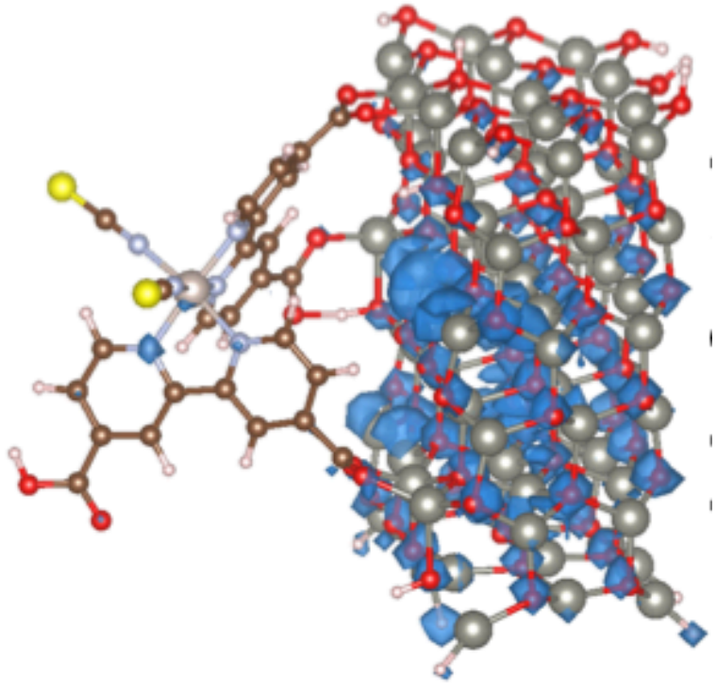
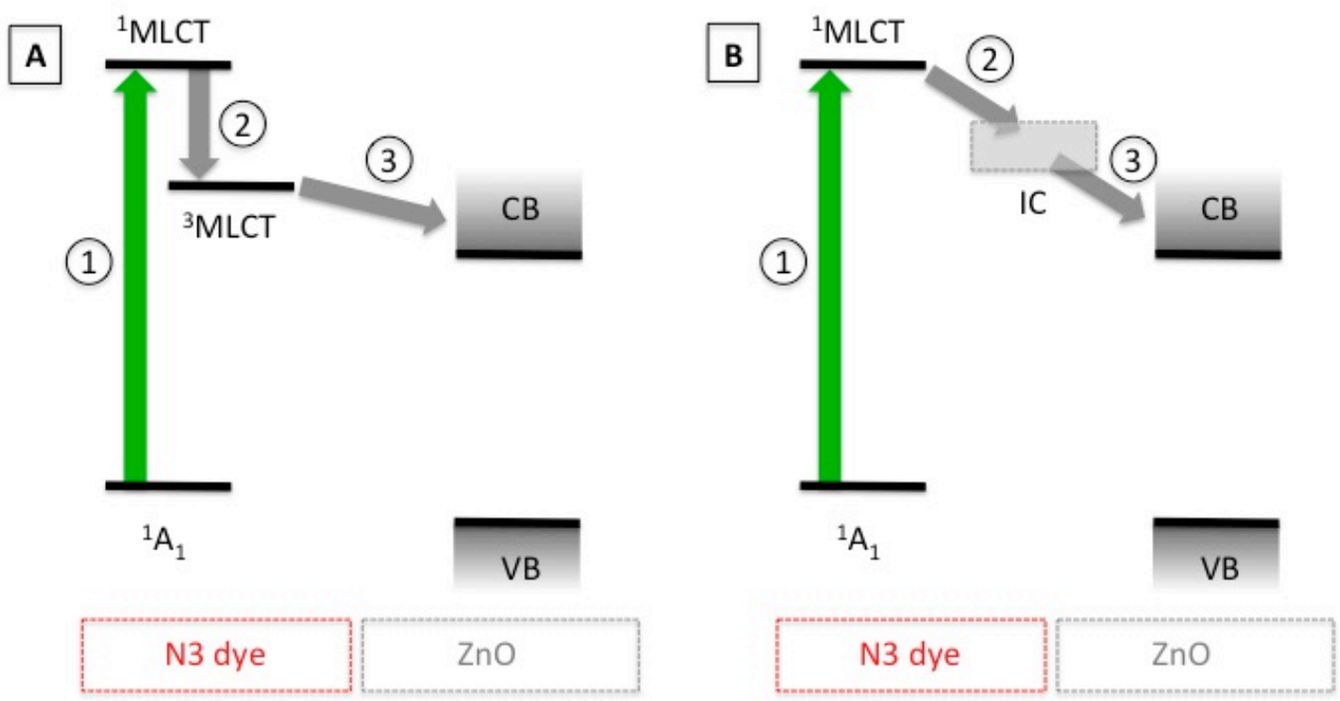
Pascal, et al. J. Phys. Chem. Lett. 2014, 5, 1547−1551

Functionalized semiconductors for solar harvesting: Dye-Sensitized Solar Cells (DSCs)



Graetzel Cell





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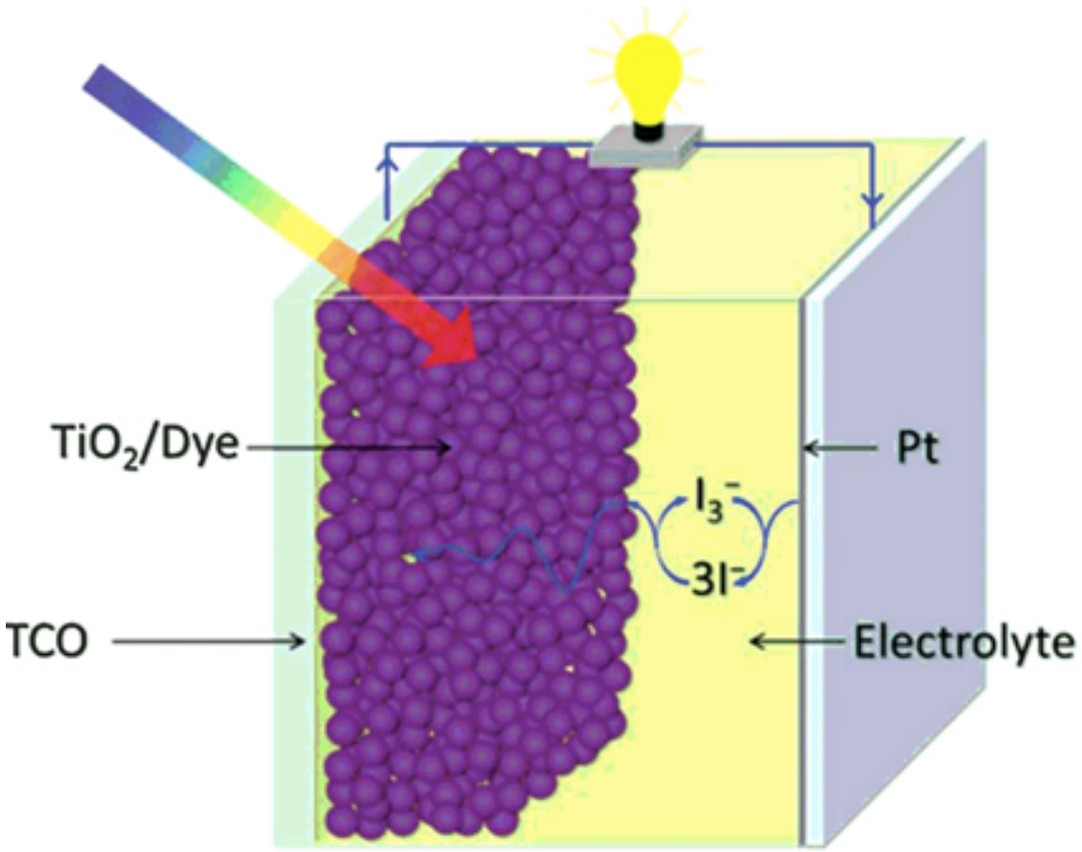
Exploring charge dynamics at the dye-substrate interface (Oliver Gessner (LBNL), Foundry User Project)



Using pump probe X-ray spectroscopy:
- explore charge state of specific atoms
- correlate with charge transfer
- extract device dynamics

Requires ultrafast light source
- X-ray Free Electron Laser (LCLS@SLAC)

Requires well controlled sample
- DSC's inherently complex

What insights can theory/simulation provide?

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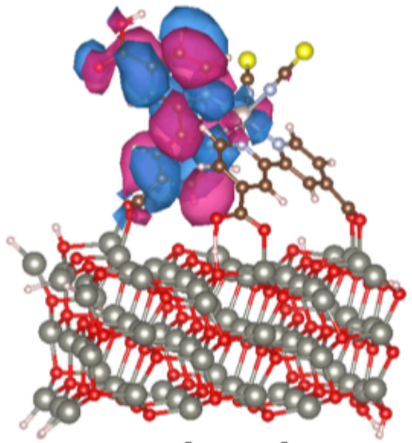
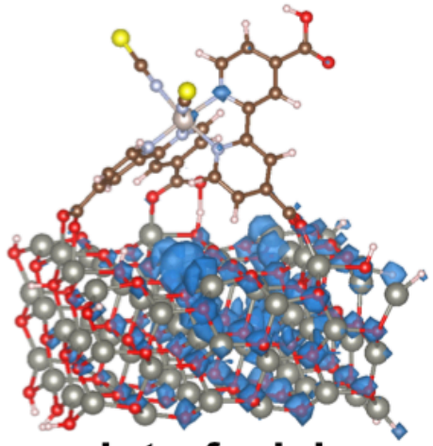
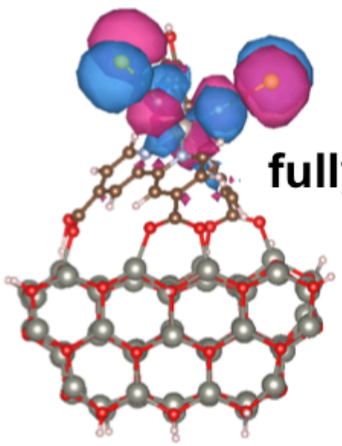
Hybrid functionals point to "Interfacial State" interpretation



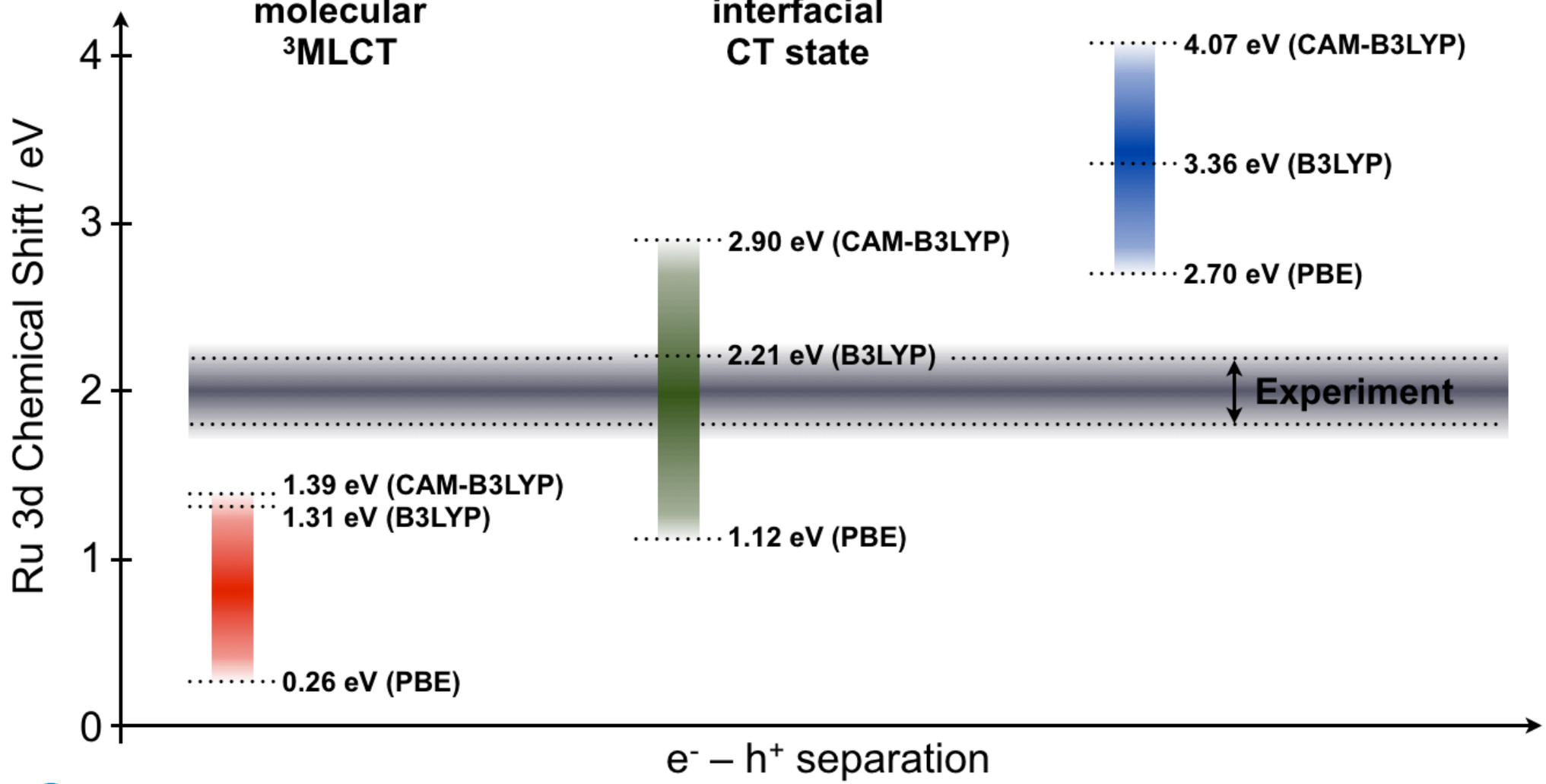
molecular
^{3}MLCT



interfacial
CT state



fully ionized



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Siefermann, Pemmaraju, Prendergast, Gessner, et al., J Phys Chem Lett (2014)

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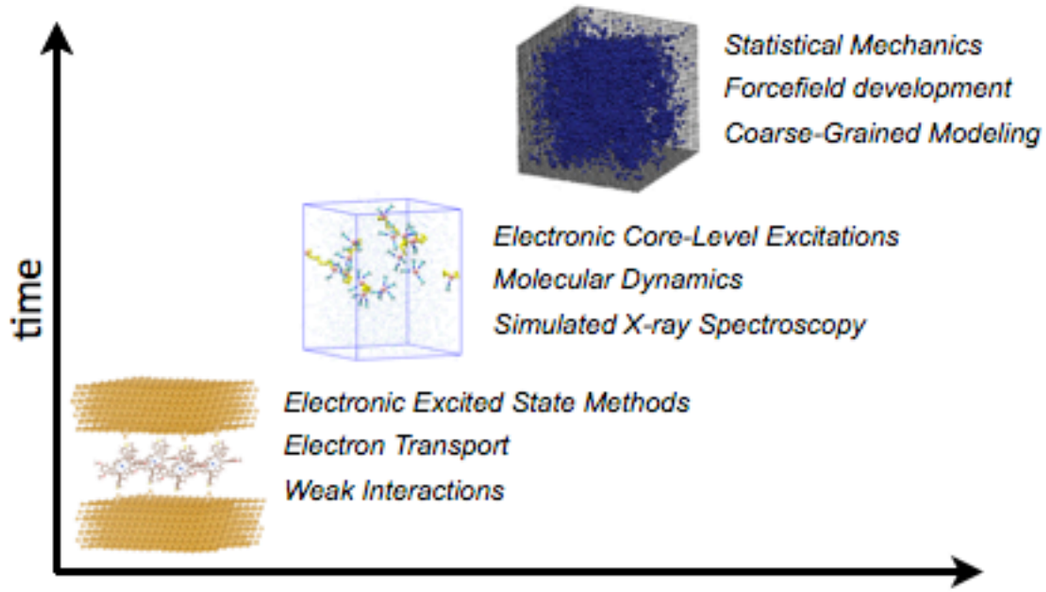
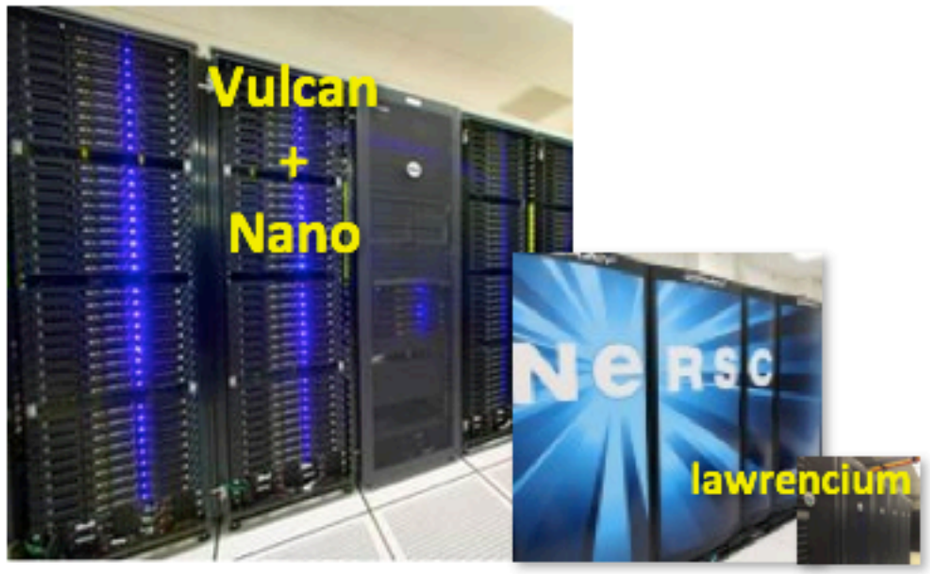
Drivers for Theory and Simulation at the Foundry

Expertise from electrons to assemblies



Computing Resources



22M CPUhr 6M <1M

Algorithmic and Use-Inspired Development

SciDAC
Scientific Discovery through Advanced Computing

BerkeleyGW

NVIDIA

MATERIALS PROJECT

EFRC
Energy Frontier Research Center
for gas separations relevant to clean air technologies

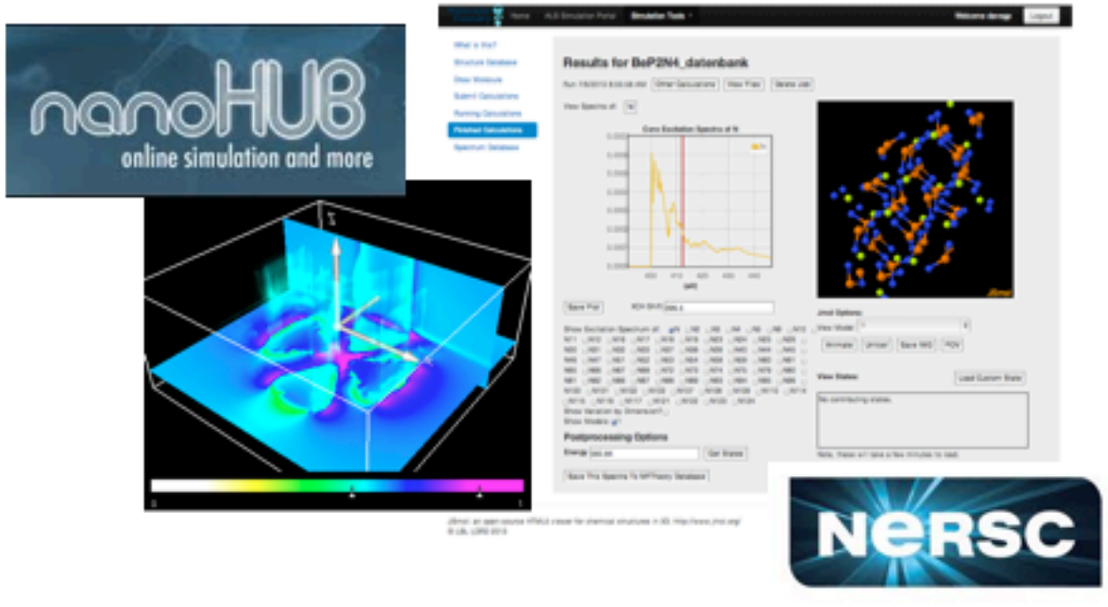
NCGC

Anodes
Cathodes
Electrolytes

JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

JCESR

Online Tools and Web-based HPC

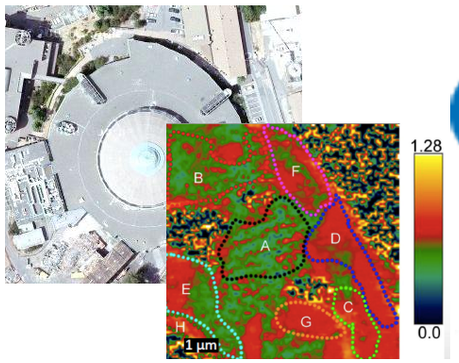


User Support/High Throughput

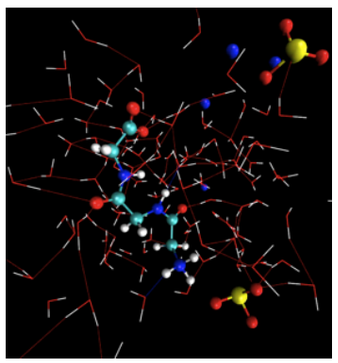
Web-based tools

Goal: To enhance User experience and throughput by providing access to unique computational tools running on high performance computing (HPC) resources

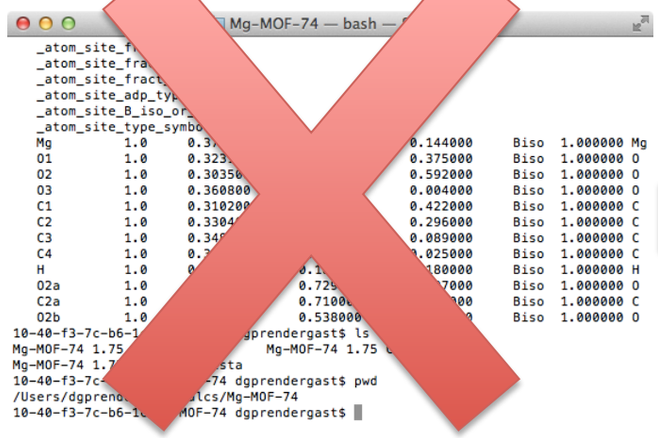
Specific Tool: WebXS – interpretation of X-ray absorption spectra



FIZ Karlsruhe ICSD



Unix/Terminal access



HPC/Cloud resources

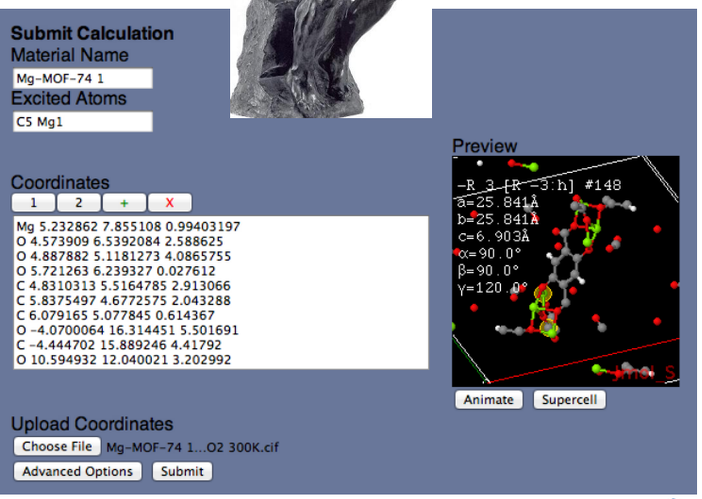
Molecular Foundry

BERKELEY LAB

Web-based tools

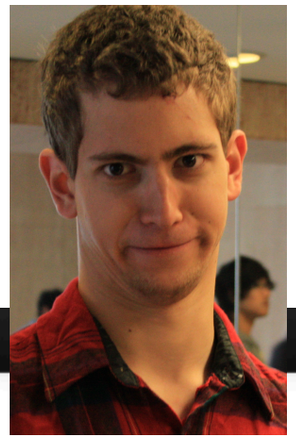
Goal: To enhance User experience and throughput by providing access to unique computational tools running on high performance computing (HPC) resources

Specific Tool: WebXS – interpretation of X-ray absorption spectra



Molecular Foundry

BERKELEY LAB



James Wonsever

WebXS
X-ray Spectra Analysis

newt
https://newt.nersc.gov/

NERSC
National Energy Research Scientific Computing Center

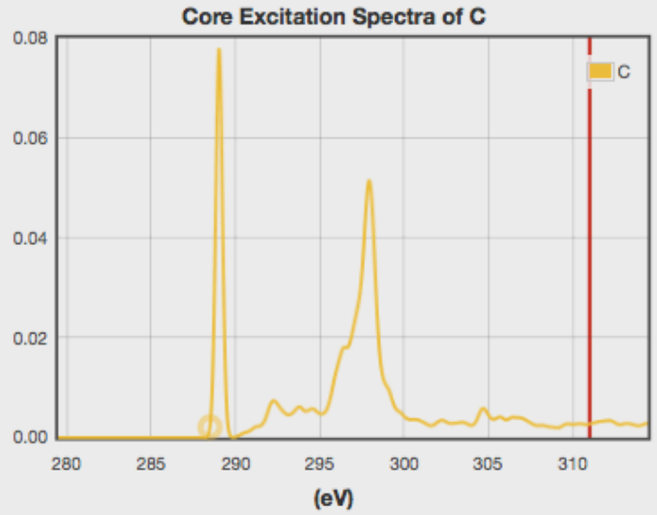
Molecular Foundry | Home | ALS Simulation Portal | Simulation Tools | Welcome davegp | Logout

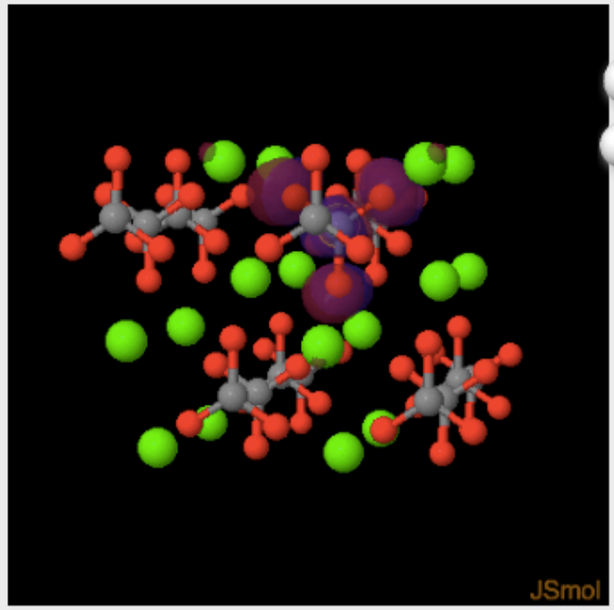
- What is this?
- Structure Database
- Draw Molecule
- Submit Calculations
- Running Calculations
- Finished Calculations
- Spectrum Database

Results for aragonite_de_Villiers-212

Run Fri Dec 27 01:45:45 2013 | Other Calculations | View Files | Delete Job

View Spectra of: C





JSmol
http://sourceforge.net/projects/jsmol/

Flot
http://www.flotcharts.org/

Save Plot | XCH Shift: 284.5

Show Excitation Spectrum of: C C17 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C30 C31 C32

Show Variation by Dimension?

Show Models: 1

Postprocessing Options

Energy 302.15 | Get States

Save This Spectra To MFTheory Database

Jmol Options:

View Model 1

Animate | Unitcell | Save IMG | POV

View States: Load Custom State

Atom|Model|State|Ev|Str		
C32|1|257|289.03|22.6951	Run	View
C30|1|257|289.03|22.69477	Run	View
C29|1|257|289.03|22.6947	Run	View

HTML5/javascript
jQuery, AJAX, php

Molecular Foundry

https://portal.nersc.gov/project/mftheory/webtools/WebXS/index.php

http://portal.hpcs.lbl.gov/webtools/WebXS

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